Relativistic Configuration-Interaction Calculations of the n=3-3 Transition Energies in Highly-Charged Tungsten Ions

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Relativistic configuration-interaction calculations of the $n = 3 - 3$ transition energies in highly-charged tungsten ions

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A large-scale relativistic configuration-interaction (CI) calculation of the $n = 3 - 3$ transition energies for Ne- to Ar-like tungsten is carried out. The calculation is based on the relativistic no-pair Hamiltonian and uses finite B-spline orbitals in a cavity as basis functions. Quantum electrodynamic and mass polarization corrections are also included. Results are compared with other theories and with experiment, and are generally found to be more reliable than previous theoretical predictions.

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I. INTRODUCTION

Tungsten is of interest in fusion research as it is a promising wall material in future magnetic confinement fusion reactors such as the International Thermonuclear Experimental Reactor (ITER) due to its desirable properties with low hydrogen retention, high melting point and high thermal conductivity. However, since tungsten is a high-Z element, even with 10 - 20 KeV reactor temperature, line emission in the x-ray and vacuum ultraviolet (VUV) regions are major concerns in realizing the magnetically confined fusion reactors. To understand its influence as a plasma impurity, reliable transition energy data are needed for many ionic stages of tungsten which show up in relevant emission spectra.

There are not many experimental and theoretical studies in the literature for the $n = 3 - 3$ transition energies of highly-charged tungsten ions. Early calculations of the sodium isoelectronic sequence are mostly based on the Dirac-Fock (DF) [1–3] or model potential [4] methods with a relatively crude accuracy of a few eV. High-precision relativistic many-body perturbation theory (RMBPT) calculations of the correlation energies for selected Na-like ions were carried out by Johnson et al. [5], but quantum electrodynamic (QED) corrections, which are important for high-Z ions, were not included. Kim et al. [6] later used these RMBPT results to provide accurate relativistic correlation corrections to their DF energies for Na-like ions with $14 \leq Z \leq 92$, and calculated the QED corrections with the ad hoc Welton method [7]. Reliable QED corrections from ab initio calculations were first given by Blundell [8] who added them to the RMBPT energies [5] to give accurate transition energies for a few Na-like ions, though tungsten was not included. Theoretical $n = 3 - 3$ resonance line energies for Mg-like ions include results from the multiconfiguration Dirac-Fock (MCDF) calculations by Cheng and Johnson [9] and Zou and Froese-Fischer [10], the

relativistic random-phase approximation calculations by Shorer et al. [11], the relativistic perturbation calculations with model potentials by Ivanova et al. [12], and the relativistic configuration-interaction (RCI) calculations for low- to mid-Z ions by Chen and Cheng [13]. For the aluminum isoelectronic sequence, transition energies and radiative rates have been calculated with the MCDF method by Huang [14] and the RMBPT method by Safronova et al. [15]. In other Al-like calculations [16–18], either tungsten is not included or results are presented in graphical forms only. Finally, there is a recent RMBPT study of wavelengths and transition rates in several highly-charged tungsten ions, including Mg- and Al-like tungsten, by Safronova and Safronova [19].

On the experimental front, there are very few measurements of the $n = 3 - 3$ wavelengths of highly-charged tungsten ions. Ralchenko et al. [20] measured EUV spectra from calciumlike W^{54+} to sodiumlike W^{63+} at the National Institute of Standards and Technology (NIST) electron beam ion trap (EBIT) facility. Gillaspy et al. [21] measured the D-line doublets in highly-charged Na-like ions as well as the wavelengths for several transitions in Si-, Al-, and Mg-like ions, including tungsten ions, at the same facility. Recently, Clementson and Beiersdorfer [22] measured $3s_{1/2}-3p_{3/2}$ and $3p_{1/2}-3d_{3/2}$ wavelengths in potassiumlike W^{55+} through neonlike W^{64+} ions at the Lawrence Livermore National Laboratory EBIT facility. The experiment relies on the calculations of the Flexible Atomic Code (FAC) [23] for line identifications. The FAC is a relativistic configuration-interaction code with Dirac-Hartree-Slater basis functions. It uses the long-wavelength approximation for the Breit energy and obtains screened QED corrections from the hydrogenic values [24, 25] by simple Z-scalings. Clementson and Beiersdorfer also calculated the transition energies with the GRASP code [26] which is based on the MCDF method, with similar QED corrections as those from the FAC.

While FAC and GRASP are invaluable for line identifications, neither of them are high-precision calculations. In the past, we have carried out accurate RCI calculations with ab initio QED corrections for a few $3s - 3p_{3/2}$ transition energies of Na-, Mg-, Al- and Si-like uranium with much smaller CI expansions and results are in excellent

agreement with measurements [27]. We shall use similar methods to calculate the $n = 3 - 3$ transition energies of some of the measured x-ray lines in highly-charged tungsten ions. In the following two sections, we shall give a brief description of the present RCI calculations. Results are then presented and discussed in Section IV, and comparisons will be made with with other theories and with experiment. A summary will be given in the last section.

II. THEORETICAL METHOD

The details of our RCI method have been given before [28]. We shall only outline the essential points here. The calculation is based on the N-electron *no-pair* Hamiltonian [29, 30]

$$H_{\text{no-pair}} = \sum_{i=1}^{N} h_i + \Lambda_{++}(H_\text{C} + H_\text{B})\Lambda_{++} \qquad (1)$$

where h_i is the one-electron Dirac Hamiltonian, H_C and H_B are the Coulomb and frequency-dependent Breit interactions, respectively, and Λ_{++} is the positive-energy projection operator for excluding the negative-energy states and preventing the appearance of electron-positron pairs in higher-order perturbation calculations which leads to the continuum dissolution problem [31] that plagues the relativistic many-electron Dirac Hamiltonian. The eigenfunction $\Psi(J^\pi M)$ of an atomic state with angular momentum (J, M) and parity π is expressed as a linear combination of the many-electron configuration-state functions $\phi(\gamma_i JM)$ such that

$$\Psi(J^\pi M) = \sum_i c_i \phi(\gamma_i JM) \qquad (2)$$

where γ_i are sets of quantum numbers representing different electronic configurations with the same parity π, and c_i are configuration mixing coefficients. Variation of the energy functional $\langle \Psi | H | \Psi \rangle$ with respect to c_i, subjected to the wavefunction normalization condition $\langle \Psi | \Psi \rangle = 1$, leads to the CI equation

$$\sum_j (H_{ij} - \lambda \delta_{ij}) c_j = 0. \qquad (3)$$

where $H_{ij} = \langle \phi_i | H | \phi_j \rangle$ are the CI matrix elements. We use one-electron B-spline basis functions for a Dirac electron moving in a model potential and confining to a finite cavity [32] to construct many-electron configuration-state functions. B-spline orbitals form finite, complete basis sets representing the bound and continuum states. They also cleanly separated into positive- and negative-energy states so that the no-pair requirement can easily be implemented by using only positive-energy B-spline orbitals. In this work, B-spline basis sets are calculated in Dirac-Kohn-Sham (DKS) potentials with cavity radii of 2.2 a.u., though results are not sensitive to these choices. The numbers of B-spline orbitals generated for each of

the angular symmetries s, $p_{1/2}$, $p_{3/2}$, ... are $n = 35$ for Na- and Mg-like ions and $n = 30$ for the others. We only use the first 20 or so B-spline orbitals in the calculations which has been found to be quite sufficient. Resulting CI expansions reach 350,000 configurations, and Davidson's method [33, 34] is used to solve the large-scale CI matrix equation for the lowest-few eigenstates.

Our theoretical energies also include contributions from the nuclear recoil and quantum electrodynamic (QED) corrections. Recoil corrections for the $n = 3 - 3$ transitions are small and consist of the normal mass shifts and specific mass shifts. The former are implicitly included by the use of the finite-mass Rydberg constant in converting energies from atomic units to eV, while the later are approximately given by the mass polarization (MP) corrections which are calculated as expectation values of the operator $H_{\text{MP}} = \frac{1}{M} \sum_{i<j} \mathbf{p_i} \cdot \mathbf{p_j}$, where M is the nuclear mass, using RCI eigenfunctions. As for the QED corrections, we start by evaluating one-electron self-energy and vacuum polarization corrections. Leading vacuum polarization corrections are calculated as expectation values of the Uehling potential. Wickmann-Kroll corrections [35], like the self-energies [36], are computed non-perturbatively to all orders of $Z\alpha$. To account for screening and relaxation corrections, one-loop QED energies are calculated in DKS potentials specific to the valence configurations of the initial and final states. The sums of the one-electron QED corrections, weighted by the effective occupation numbers from the RCI calculations, give the many-electron QED energies. Corrections from higher-order two-loop Lamb shifts are also included. They are small and are order-of-magnitude estimates only.

III. CI EXPANSIONS

The fourteen $n = 3 - 3$ transition lines considered here are listed in Table I. For the ten lines that are measured in [22], we use the same line labels there consisting of an isoelectronic identifier followed by an integer (Na-1, Mg-2, etc.). For the other four lines measured in [20], we use similar line labels, but with the trailing integer replaced by a Greek alphabet as in Na-α, Mg-β, Al-γ and Al-δ. For each of these lines, we start by defining reference configurations for the upper and lower states consisting of core and valence electrons. Single and double excitations of at least one valence electron and up to one core electron from these reference configurations are then included in the CI expansions to account for valence-valence (VV) and core-valence (CV) correlations. In the case of Na-like ions, core-core (CC) correlations with the excitations of two core electrons are also included. Descriptions of the CI expansions are given in the following. For brevity, the $1s^2$ core is omitted unless it is explicitly involved in the excitations.

1) For the Ne-1 line of W^{64+}, the reference states are $2s^2 2p_{1/2}^2 2p_{3/2}^3 3\bar{l} + 2s^2 2p_{1/2} 2p_{3/2}^4 3\bar{l}$, with the F-like $2s^2 2p^5$

TABLE I: Spectral lines studied in this work. The F-like core is the $1s^2 2s^2 2p^5$ $J^\pi = 3/2^-$ state. The Ne-like core is the $1s^2 2s^2 2p^6$ $J^\pi = 0^+$ state. Upper and lower state identifications are given by core + the respective valence configurations.

Ion	Line	Core	J^π_{core}	Lower state	J^π_{lower}	Upper state	J^π_{upper}
W^{64+}	Ne-1	F-like	$3/2^-$	$3s$	1^-	$3p_{3/2}$	0^+
W^{63+}	Na-1	Ne-like	0^+	$3s$	$1/2^+$	$3p_{3/2}$	$3/2^-$
	Na-α	Ne-like	0^+	$3s$	$1/2^+$	$3p_{1/2}$	$1/2^-$
W^{62+}	Mg-2	Ne-like	0^+	$3s^2$	0^+	$3s3p_{3/2}$	1^-
	Mg-β	Ne-like	0^+	$3s^2$	0^+	$3s3p_{1/2}$	1^-
W^{61+}	Al-1	Ne-like	0^+	$3s^2 3p_{1/2}$	$1/2^-$	$3s^2 3d_{3/2}$	$3/2^+$
	Al-2	Ne-like	0^+	$3s^2 3p_{1/2}$	$1/2^-$	$3s3p_{1/2}[1]3p_{3/2}$	$1/2^+$
	Al-3	Ne-like	0^+	$3s^2 3p_{1/2}$	$1/2^-$	$3s3p_{1/2}[1]3p_{3/2}$	$3/2^+$
	Al-4	Ne-like	0^+	$3s^2 3p_{1/2}$	$1/2^-$	$3s3p_{1/2}[0]3p_{3/2}$	$3/2^+$
	Al-γ	Ne-like	0^+	$3s^2 3p_{1/2}$	$1/2^-$	$3s3p^2_{1/2}$	$1/2^+$
	Al-δ	Ne-like	0^+	$3s3p^2_{1/2}$	$1/2^+$	$3s^2 3p_{3/2}$	$3/2^-$
W^{60+}	Si-1	Ne-like	0^+	$3s^2 3p^2_{1/2}$	0^+	$3s^2 3p_{1/2} 3d_{3/2}$	1^-
	Si-2	Ne-like	0^+	$3s^2 3p^2_{1/2}$	0^+	$3s3p^2_{1/2} 3p_{3/2}$	1^-
W^{56+}	Ar-1	Ne-like	0^+	$3s^2 3p^6$	0^+	$3s^2 3p_{1/2} 3p^4_{3/2} 3d_{3/2}$	1^-

core and $3\bar{l} = 3s, 3p$ valence electrons. The CI expansions from valence excitations and CV correlations between the $n = 2$ and $n = 3$ shells include the configurations $2s^2 2p^5 nl$, $2s^2 2p^4 nln'l'$ and $2s2p^5 nln'l'$. One- and two-electron excitations are limited to $n, n' \le 20$ and $l, l' \le 3$.

2) For the Na-1 and Na-α lines of W^{63+}, the reference states are $1s^2 2s^2 2p^6 3\bar{l}$ with the Ne-like core and $3\bar{l} = 3s, 3p$ valence electrons. The basic CI expansions from valence excitations and CV correlations arising from single- and double-excitations of the $1s$, $2s$, $2p$ core and $3\bar{l}$ valence electrons include the configurations $1s^2 2s^2 2p^6 nl$, $1s^2 2s^2 2p^5 nln'l'$, $1s^2 2s 2p^6 nln'l'$ and $1s2s^2 2p^6 nln'l'$, with $n, n' \le 23$ and $l, l' \le 5$. We also includes CC correlations from the $n = 2$ subshells with the configurations $1s^2 2s^2 2p^4 3\bar{l}nln'l'$, $1s^2 2s2p^5 3\bar{l}nln'l'$ and $1s^2 2p^6 3\bar{l}nln'l'$, with $n, n' \le 23$, and $l, l' \le 3$. The reduced basis sets are adequate for the small CC corrections and help keep the sizes of these large-scale CI calculations manageable.

3) For the Mg-2 and Mg-β lines of W^{62+}, the reference states are the Ne-like core plus $3s^2 + 3p^2$ for the lower state and $3s3p + 3p3d$ for the upper state. With $3\bar{l} = 3s, 3p$ and $3s, 3p, 3d$ for the lower and upper states, respectively, the CI expansions include VV correlations $(2s^2 2p^6 nln'l')$ and CV correlations from the $n = 2$ core and $n = 3$ valence shells $(2s^2 2p^5 3\bar{l}nln'l', 2s2p^6 3\bar{l}nln'l')$ with $n, n' \le 22$ and $l, l' \le 5$. No CC correlation is included.

4) For the six Al-like lines of W^{61+}, the core is again the Ne-like ground state, while the three valence electrons are from the $3s, 3p$ shells, except for the upper states of Al-1 which are from the $3s, 3d$ shells. The basic CI expansions include VV and CV correlations from the $n = 2$ core and the $n = 3$ valence shells with $n \le 20$ and $l \le 5$, except for Al-3 and Al-4 where $n \le 18$ and $l \le 3$.

5) For the Si-1 and Si-2 lines of W^{60+}, the reference states consist of the Ne-like core with four valence electrons from the $3\bar{l} = 3s, 3p$ subshells for the lower states

and $3\bar{l} = 3s, 3p, 3d$ and $3s, 3p$ subshells for the upper states of Si-1 and Si-2, respectively. We consider VV correlations only with the excitations of up to two valence electrons to $3\bar{l}3\bar{l}'nln'l'$ states, with $n, n' \le 20$ and $l, l' \le 5$.

6) For the Ar-1 line of W^{56+}, the core is the Ne-like ground state and valence shells are $3s, 3p$ for the lower state and $3s, 3p, 3d$ for the upper state. CI expansions again include VV correlations only with $n \le 18$ and $l \le 5$.

IV. RESULTS AND DISCUSSION

In Table II, contributions to the transition energies of the fourteen $n = 3 - 3$ tungsten lines are shown. They include Coulomb and frequency-dependent Breit energies from the present RCI calculations, along with the mass polarization and QED corrections which are also calcu-

TABLE II: Contributions (eV) from Coulomb, Breit, MP, and QED to the $n = 3 - 3$ transition energies for tungsten ions. Numbers in parentheses are error estimates.

Line	Coulomb	Breit	MP	QED	Total
Ne-1	590.68(5)	1.71	-0.01	-4.50(5)	587.88(7)
Na-1	538.01(3)	-0.50	-0.01	-4.41(4)	533.09(5)
Na-α	160.24(3)	4.13	-0.01	-4.85(4)	159.51(5)
Mg-2	550.13(5)	-0.52	-0.01	-4.34(5)	545.27(7)
Mg-β	156.00(5)	3.81	-0.01	-4.75(5)	155.05(7)
Al-1	602.39(30)	-4.65	0.00	-1.17(2)	596.57(30)
Al-2	554.60(10)	-0.27	-0.01	-4.32(5)	550.00(11)
Al-3	544.96(30)	-1.68	-0.01	-3.62(4)	539.65(30)
Al-4	505.19(30)	-0.31	-0.01	-4.27(5)	500.60(30)
Al-γ	167.95(10)	4.24	-0.01	-4.73(5)	167.45(11)
Al-δ	199.66(10)	-8.67	-0.01	5.11(5)	196.09(11)
Si-1	618.22(40)	-4.65	-0.01	-1.06(2)	612.47(40)
Si-2	549.12(40)	-1.35	0.00	-3.61(4)	544.16(40)
Ar-1	636.67(50)	-5.41	0.00	-0.37(1)	630.89(50)

TABLE III: Comparison between theory and experiment for the $n = 3 - 3$ transition energies of tungsten ions. Numbers in parentheses are theoretical and experimental uncertainties.

Line	RCI[a]	FAC[b]	GRASP[b]	RMBPT[c]	Expt[b]
Ne-1	587.88(7)	591.27	591.10		588.02(17)
Na-1	533.09(5)	533.56	533.38	533.08[d]	533.20(11)
Na-α	159.51(5)	159.74[e]		159.50[d]	159.59(4)[e]
Mg-2	545.27(7)	546.16	544.87	545.90	545.35(10)
Mg-β	155.05(7)	155.17[e]		155.25	155.15(4)[e]
Al-1	596.57(30)	598.35	600.79		597.34(12)
Al-2	550.00(11)	550.89	552.76		549.99(10)
Al-3	539.65(30)	540.24	542.48		539.98(14)
Al-4	500.60(30)	500.54	499.65		500.3(2)
Al-γ	167.45(11)	167.65[e]		167.37	167.46(5)[e]
Al-δ	196.09(11)	196.03[e]		195.97	196.24(9)[e]
Si-1	612.47(40)	612.90	613.78		611.66(15)
Si-2	544.16(40)	544.60	544.65		543.96(12)
Ar-1	630.89(50)	631.41	632.35		630.03(22)

[a]This work.
[b]Clememtson and Beiersdorfer [22] unless otherwise specified.
[c]Safronova and Safronova [19] unless otherwise specified.
[d]Sapirstein and Cheng, [37].
[e]Ralchenko et al. [20].

lated here. The ten lines with labels ending in an integer (Na-1, Mg-2, etc.) have energies ranging from 500 – 640 eV. They are from the $3s_{1/2} - 3p_{3/2}$ and $3p_{1/2} - 3d_{3/2}$ transitions which, in the high-Z jj-coupling limit, are very close in energy. The remaining four lines with labels ending in a Greek alphabet (Na-α, Mg-β, Al-γ, Al-δ) are from the $3s_{1/2} - 3p_{1/2}$ transitions with lower energies of 150 – 200 eV.

Transition energies are dominated by the Coulomb energies, with large corrections from the Breit and QED corrections for these high-Z ions. While the Breit energies depend on the details of the electronic configurations and vary in magnitude from 0.27 to 8.67 eV, most of the QED corrections are about -4.5 eV in size as they are dominate by the QED energy of the $3s$ electron in $3s - 3p$ transitions. Exceptions are the Al-1, Si-1 and Ar-1 lines which are $3p_{1/2} - 3d_{3/2}$ transitions and QED corrections are substantially smaller at -1.17, -1.06 and -0.37 eV, respectively. In all cases, mass polarization corrections are very small at about -0.01 eV and are quite negligible.

We note that to keep the sizes of the CI expansions computationally manageable, most of the RCI results only included VV and CV correlations from single and double excitations from the reference states, and some with VV correlations only. For the Na-like tungsten ions, however, CC correlations from the $1s$, $2s$ and $2p$ subshells are also included. They amount to -0.03 and 0.02 eV corrections to the Coulomb energies for the Na-1 and Na-α lines, respectively. Furthermore, with the choices of the reference states here, we found that it is important to include triple excitations in our RCI calculations of the Al-1 and Al-3 lines. Specifically, for the $3s^2 3d$ $J=3/2$ upper state in Al-1, we in-

clude the configurations $2s^2 2p^6 3pnln'l'$, $2s^2 2p^5 3s3pnln'l'$ and $2s2p^6 3s3pnln'l'$. For the $3s3p_{1/2}[1]3p_{3/2}$ $J=3/2$ upper state in Al-3, we include the configurations $2s^2 2p^5 3s^2 nln'l'$, $2s^2 2p^5 3s3dnln'l'$, $2s2p^6 3s^2 nln'l'$ and $2s2p^6 3s3dnln'l'$. For these two lines, corrections from triple excitations reduce the transition energies by 1.89 and 0.84 eV, respectively.

In Table III, the $n = 3 - 3$ transition energies for tungsten ions are compared between theories and experiments. Theoretical energies relative to experimental energies are also plotted in Fig. 1. It can be seen that the present RCI results are more accurate than those of FAC and GRASP. For the Na-1 and Na-α lines, our RCI energies are in excellent agreement with the RMBPT results of Sapirstein and Cheng [37], both are in good agreement with experiment and have the same QED corrections from ab initio calculations outlined earlier. For the $3s - 3p_{1/2}$ Mg-β , Al-γ and Al-δ lines, our RCI energies are also in good agreement with the RMBPT results of Safronova and Safronova [19], though with larger discrepancies up to 0.2 eV which are likely due to differences in QED corrections: While our QED energies are directly calculated, those in [19] are scaled from the Na-like QED results of Blundell [8] for the Mg-β line, and from Mohr's hydrogenic results [24, 25] with ad hoc screening corrections for the Al-γ and Al-δ lines. For the $3s - 3p_{3/2}$ Mg-2 line, however, the RMBPT result of [19] is higher

FIG. 1: (Color online) Theoretical energies relative to the experimental energies. Solid circles are the present RCI results. Open squares and crosses are RMBPT results of [37] and [19], respectively. Solid triangles and open inverted triangles are FAC and GRASP results, respectively. Horizontal error bars are experimental uncertainties.
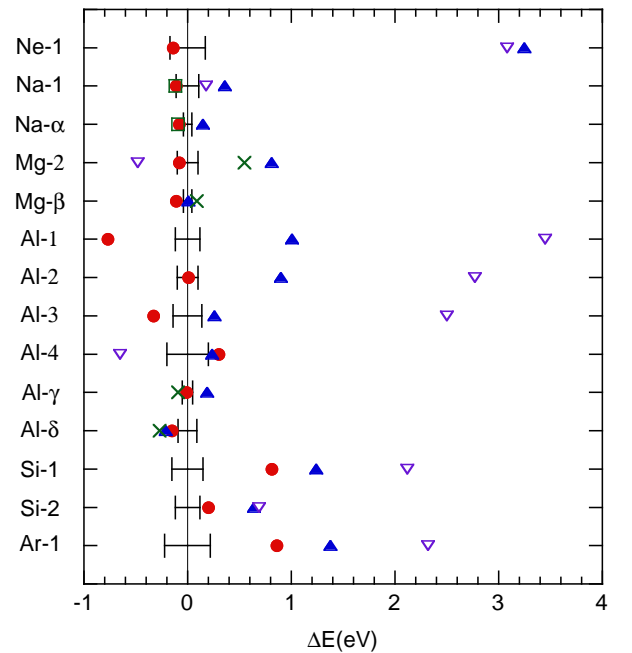
than our RCI energy, which is in good agreement with experiment, by 0.63 eV and it is not clear if this is due solely to the discrepancy in QED corrections. In general, differences between RCI and experiment go up with the numbers of $n = 3$ valence electrons, as it is increasingly more difficult to include all dominant configurations in the CI expansions. For the Al-1, Al-3 and Al-4 lines, the discrepancies are likely due to inadequate treatment of triple excitations. For the Si-1, Si-2 and Ar-1 lines, they probably come from the lack of CV correlations as we are limited by the sizes of the RCI calculations to VV correlations only.

V. SUMMARY

We have calculated the $n = 3-3$ transition energies for highly-charged tungsten ions from Ne- to Ar-like systems using a large-scale RCI method. QED corrections including screening and relaxation effects are also included. Our results are generally in very good agreement with experiments, though theoretical accuracies are clearly limited by the sizes of CI expansions. Nevertheless, these computational constrains can be overcome with more efficient and compact basis sets as well as faster and more capable computers. Tungsten is of great interests in fusion reactor designs and it is desiable to have more precision measurements of the $n = 3-3$ as well as $n = 2-2$ transitions in highly-charged tungsten ions.

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